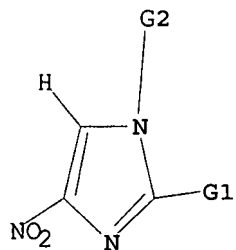


=> d l1

L1 HAS NO ANSWERS

L1 STR



1 S — Cb

G1 X, [01]

G2 C, H

Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 12:05:36 ON 25 APR 2007)

FILE 'REGISTRY' ENTERED AT 12:06:04 ON 25 APR 2007

L1 STRUCTURE UPLOADED

L2 QUE L1

L3 17 S L1

L4 320 S L1 FUL

L5 289 S L4 AND CAPLUS/LC

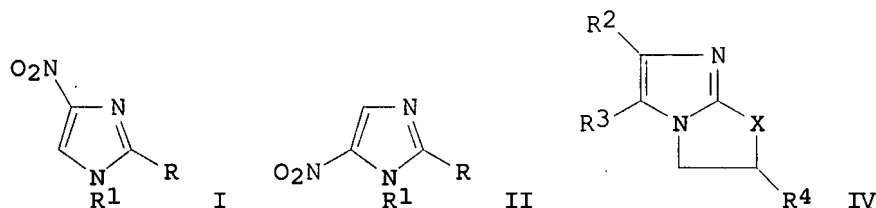
L6 31 S L4 NOT L5

FILE 'ZCAPLUS' ENTERED AT 12:08:18 ON 25 APR 2007

L7 52 S L4

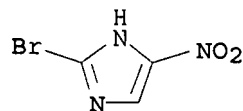
*SS*  
4/25/07

L8 ANSWER 4 OF 52 ZCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1984:611044 ZCAPLUS <<LOGINID::20070425>>  
 DOCUMENT NUMBER: 101:211044  
 TITLE: Nitroimidazoles: part XX - reactions of  
 2,4-dinitroimidazole with 2-haloethanols,  
 3-chloropropionitrile and propylene oxide  
 AUTHOR(S): Nagarajan, K.; Shenoy, S. J.  
 CORPORATE SOURCE: Res. Cent., CIBA-GEIGY, Bombay, 400 063, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic  
 Chemistry Including Medicinal Chemistry (1984),  
 23B(4), 363-8  
 CODEN: IJSBDB; ISSN: 0376-4699  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 101:211044  
 GI



AB 2,4-Dinitroimidazoles I (R = NO<sub>2</sub>, R<sub>1</sub> = Me) reacted with BrCH<sub>2</sub>CH<sub>2</sub>OH, ClCH<sub>2</sub>CH<sub>2</sub>OH, Cl(CH<sub>2</sub>)<sub>3</sub>OH or ClCH<sub>2</sub>CH<sub>2</sub>CN to give I (R = Br, Cl; R<sub>1</sub> = H, Me). Methylation of I (R = Br, Cl; R<sub>1</sub> = H) gave isomeric imidazoles I and II (R = Br, Cl; R<sub>1</sub> = Me). Other products from the reaction of I (R = NO<sub>2</sub>, R<sub>1</sub> = H) (III) and ClCH<sub>2</sub>CH<sub>2</sub>CN were I (R = Cl, R<sub>1</sub> = CH<sub>2</sub>CH<sub>2</sub>CN, CH<sub>2</sub>CH<sub>2</sub>CONH<sub>2</sub>) and cyclocondensation product pyrroloimidazole IV (R<sub>2</sub> = NO<sub>2</sub>, R<sub>3</sub> = R<sub>4</sub> = H; X = CO). III reacted with propylene oxide to give imidazooxazoline IV (R<sub>2</sub> = H, R<sub>3</sub> = NO<sub>2</sub>, R<sub>4</sub> = Me; X = O) and I (R = NO<sub>2</sub>, R<sub>1</sub> = CH<sub>2</sub>CHMeOH, CHMeCH<sub>2</sub>OH), which (R<sub>1</sub> = CH<sub>2</sub>CHMeOH) cyclized to give IV (R<sub>2</sub> = NO<sub>2</sub>, R<sub>3</sub> = H, R<sub>4</sub> = Me; X = O). Propylene oxide and I (R = Cl, R<sub>1</sub> = H) gave I and II (R = Cl, R<sub>1</sub> = CH<sub>2</sub>CHMeOH), the latter of which cyclized to give IV (R<sub>2</sub> = H, R<sub>3</sub> = NO<sub>2</sub>, R<sub>4</sub> = Me; X = O).

IT **65902-59-2P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and methylation of)  
 RN 65902-59-2 ZCAPLUS  
 CN 1H-Imidazole, 2-bromo-4-nitro- (9CI) (CA INDEX NAME)

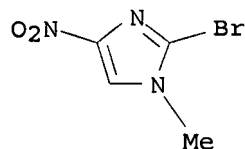


IT 16681-63-3P 63634-21-9P 92918-17-7P  
92918-18-8P 92918-22-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

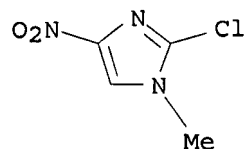
RN 16681-63-3 ZCAPLUS

CN 1H-Imidazole, 2-bromo-1-methyl-4-nitro- (9CI) (CA INDEX NAME)



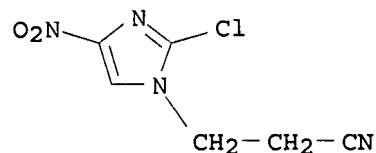
RN 63634-21-9 ZCAPLUS

CN 1H-Imidazole, 2-chloro-1-methyl-4-nitro- (9CI) (CA INDEX NAME)



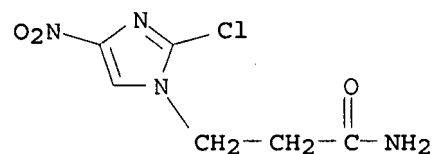
RN 92918-17-7 ZCAPLUS

CN 1H-Imidazole-1-propanenitrile, 2-chloro-4-nitro- (9CI) (CA INDEX NAME)



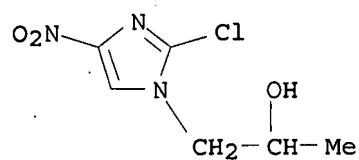
RN 92918-18-8 ZCAPLUS

CN 1H-Imidazole-1-propanamide, 2-chloro-4-nitro- (9CI) (CA INDEX NAME)



RN 92918-22-4 ZCAPLUS

CN 1H-Imidazole-1-ethanol, 2-chloro- $\alpha$ -methyl-4-nitro- (9CI) (CA INDEX NAME)



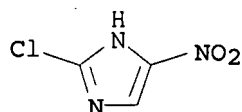
IT **57531-37-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

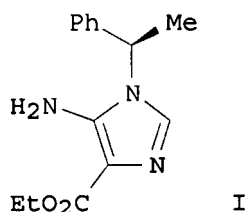
(preparation, methylation, and alkylation of, with propylene oxide)

RN 57531-37-0 ZCAPLUS

CN 1H-Imidazole, 2-chloro-5-nitro- (CA INDEX NAME)



L8 ANSWER 6 OF 52 ZCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:246882 ZCAPLUS <<LOGINID::20070425>>  
DOCUMENT NUMBER: 139:69198  
TITLE: Synthesis of chiral imidazole derivatives as purine precursors  
AUTHOR(S): Suwinski, Jerzy; Szczepankiewicz, Wojciech; Swierczek, Krzysztof; Walczak, Krzysztof  
CORPORATE SOURCE: Institute of Organic Chemistry and Technology, Silesian University of Technology, Gliwice, Pol.  
SOURCE: European Journal of Organic Chemistry (2003), (6), 1080-1084  
CODEN: EJOCFK; ISSN: 1434-193X  
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:69198  
GI



AB From com. available chiral building blocks, we have developed methods for the syntheses of imidazoles, e.g., I, that contain a chiral alkyl substituent at a ring atom. These compds. are suitable for further transformation into N-alkyl purine derivs.

IT 181022-34-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of (dihydroxypropyl)nitroimidazoles via addition of DBU-salts of nitroimidazoles to (hydroxymethyl)oxirane as purine precursors)

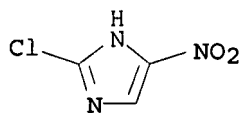
RN 181022-34-4 ZCAPLUS

CN Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro-, compd. with 2-chloro-4-nitro-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 57531-37-0

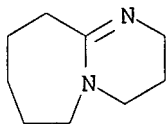
CMF C3 H2 Cl N3 O2



CM 2

CRN 6674-22-2

CMF C9 H16 N2

IT 549549-01-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

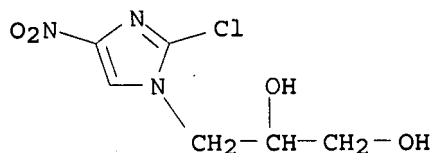
(preparation of (dihydroxypropyl)nitroimidazoles via addition of DBU-salts

of

nitroimidazoles to (hydroxymethyl)oxirane as purine precursors)

RN 549549-01-1 ZCAPLUS

CN 1,2-Propanediol, 3-(2-chloro-4-nitro-1H-imidazol-1-yl)- (9CI) (CA INDEX NAME)

IT 549549-02-2P 549549-03-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(stereoselective preparation of (dihydroxypropyl)nitroimidazoles via

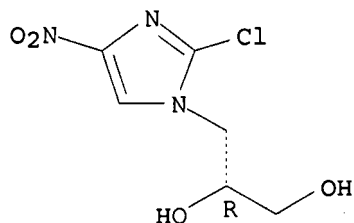
addition

of DBU-salts of nitroimidazoles to chiral (hydroxymethyl)oxirane as purine precursors)

RN 549549-02-2 ZCAPLUS

CN 1,2-Propanediol, 3-(2-chloro-4-nitro-1H-imidazol-1-yl)-, (2R)- (9CI) (CA INDEX NAME)

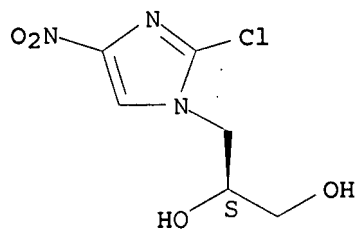
Absolute stereochemistry. Rotation (+).



RN 549549-03-3 ZCAPLUS

CN 1,2-Propanediol, 3-(2-chloro-4-nitro-1H-imidazol-1-yl)-, (2S)- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry. Rotation (-).



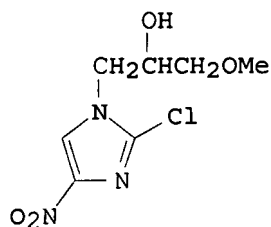
REFERENCE COUNT:

12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 20 OF 52 ZCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 1989:632816 ZCAPLUS <<LOGINID::20070425>>  
 DOCUMENT NUMBER: 111:232816  
 TITLE: Preparation of 2-chloro-1-(2-hydroxy-3-methoxypropyl)-  
 4-nitroimidazole, a sensitizer for cancer radiation  
 therapy  
 INVENTOR(S): Suwinski, Jerzy; Salwinska, Ewa; Walczak, Krzysztof;  
 Watras, Jan; Widel, Maria  
 PATENT ASSIGNEE(S): Politechnika Slaska, Pol.  
 SOURCE: Pol., 6 pp. Abstracted and indexed from the unexamined  
 application.  
 CODEN: POXXA7  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Polish  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PL 145536	B1	19880930	PL 1985-255883	19851021
PRIORITY APPLN. INFO.: GI			PL 1985-255883	19851021



AB The title compound (I) a radiation sensitizer for cancer therapy, is prepared from 2,4(5)-dinitroimidazole (II) in 2 steps: (1) reaction with boiling concentrated HCl to replace 2-NO<sub>2</sub> by 2-Cl, and (2) reaction with (methoxymethyl)oxirane (III) in the presence of K<sub>2</sub>CO<sub>3</sub> to introduce the -CH<sub>2</sub>CH(OH)CH<sub>2</sub>OMe group. Thus, 79 g II was boiled 6 h with HCl and cooled to 0° to precipitate 2-chloro-4(5)-nitroimidazole. A mixture of the latter with 6 g K<sub>2</sub>CO<sub>3</sub> and 225 mL III was stirred at 60° and worked up with aqueous crystallization to give 50-60 g (53-62%) I. Rats inoculated with Rhabdomyosarcoma R1 were irradiated 5 times/wk with a dose of 15 + 370 rad; healing efficiencies for treatment with 0.15 mg I/kg, 0.1 mg I/kg, and no I before irradiation were 83.3, 68.8, and 44.1%, resp.

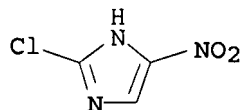
IT 57531-37-0P, 2-Chloro-4-(5)-nitroimidazole  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and alkylation of, by (methoxymethyl)oxirane)

RN 57531-37-0 ZCAPLUS

CN 1H-Imidazole, 2-chloro-5-nitro- (CA INDEX NAME)



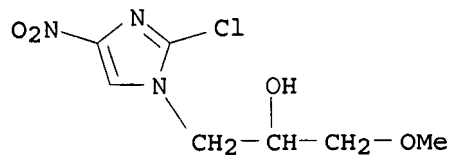


IT 111119-29-0P

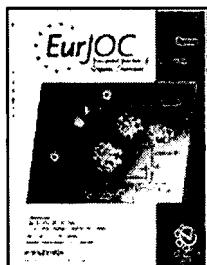
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as radiosensitizer)

RN 111119-29-0 ZCAPLUS

CN 1H-Imidazole-1-ethanol, 2-chloro- $\alpha$ -(methoxymethyl)-4-nitro- (9CI)  
(CA INDEX NAME)



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Thierry Brotin, Jean-Pierre Dutasta

Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390165

[Abstract](#) | [Full Text: PDF](#) (Size: 79K) [Save Article](#)**Graphical Abstract****Graphical Abstract:** Eur. J. Org. Chem. 6/2003 (p 925-931)

Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390166

[Abstract](#) | [Full Text: PDF](#) (Size: 217K) [Save Article](#)**Microreview****Group-IV Metal Complexes as Hydroamination Catalysts (p 935-946)**

Igor Bytschkov, Sven Doye

Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390149

[Abstract](#) | [References](#) | [Full Text: HTML, PDF](#) (Size: 303K) [Save Article](#)**Syntheses of Functionalized 2,2':6',2''-Terpyridines (p 947-961)**

Marcel Heller, Ulrich S. Schubert

Published Online: 3 Mar 2003

DOI: 10.1002/ejoc.200390150

[Abstract](#) | [References](#) | [Full Text: HTML, PDF](#) (Size: 398K) [Save Article](#)**Short Communication****A Good Bargain: An Inexpensive, Air-Stable Ruthenium Metathesis Catalyst Derived from  $\alpha$ -Asarone (p 963-966)**

Karol Grela, Mikhail Kim

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ONLINE SUBMISSION

Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390151

[Abstract](#) | [References](#) | Full Text: [HTML](#), [PDF](#) (Size: 102K)

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**Controlled Stepwise Release of Fragrance Alcohols from Dendrimer-Based 2-Carbamoylbenzoates by Neighbouring Group Participation (p 967-971)**

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Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390152

[Abstract](#) | [References](#) | Full Text: [HTML](#), [PDF](#) (Size: 113K)

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**Xe@cryptophane Complexes with C<sub>2</sub> Symmetry: Synthesis and Investigations by <sup>129</sup>Xe NMR of the Consequences of the Size of the Host Cavity for Xenon Encapsulation (p 973-984)**

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Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390153

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Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390154

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Published Online: 26 Feb 2003

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Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390141

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Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390142

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Laurence Zapata, Katell Bathany, Jean-Marie Schmitter, Serge Moreau

Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390143

[Abstract](#) | [References](#) | Full Text: [HTML](#), [PDF](#) (Size: 165K)

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Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390144

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**Sulfonate Protecting Groups: Synthesis of D- and L-myo-Inositol-1,3,4,5-tetrakisphosphate Precursors by a Novel Silver(I) Oxide-Mediated O-Alkylation of 2,4(6)-Di-O-acyl-6(4)-O-sulfonyl-myo-Inositol 1,3,5-Orthoformate Derivatives Through Intramolecular Assistance of the Sulfonyl Group (p 1035-1041)**

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Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390145

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DOI: 10.1002/ejoc.200390147

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Published Online: 26 Feb 2003

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Abstract | References | Full Text: [HTML](#), [PDF](#) (Size: 144K)

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Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390156

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Florent Allais, Rémy Angelaud, Boris Camuzat-Dedenis, Karine Julienne, Yannick Landais

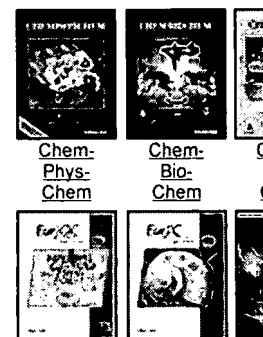
Published Online: 26 Feb 2003

DOI: 10.1002/ejoc.200390157

Abstract | References | Full Text: [HTML](#), [PDF](#) (Size: 121K)

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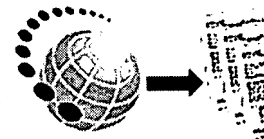


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Published Online: 26 Feb 2003

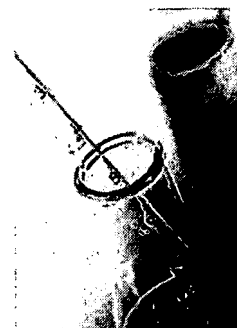
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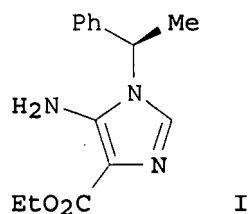
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L8 ANSWER 6 OF 52 ZCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003:246882 ZCAPLUS <<LOGINID::20070425>>  
DOCUMENT NUMBER: 139:69198  
TITLE: Synthesis of chiral imidazole derivatives as purine precursors  
AUTHOR(S): Suwinski, Jerzy; Szczepankiewicz, Wojciech; Swierczek, Krzysztof; Walczak, Krzysztof  
CORPORATE SOURCE: Institute of Organic Chemistry and Technology, Silesian University of Technology, Gliwice, Pol.  
SOURCE: European Journal of Organic Chemistry (2003), (6), 1080-1084  
CODEN: EJOCFK; ISSN: 1434-193X  
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:69198  
GI



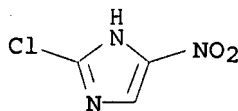
AB From com. available chiral building blocks, we have developed methods for the syntheses of imidazoles, e.g., I, that contain a chiral alkyl substituent at a ring atom. These compds. are suitable for further transformation into N-alkyl purine derivs.

IT 181022-34-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of (dihydroxypropyl)nitroimidazoles via addition of DBU-salts of nitroimidazoles to (hydroxymethyl)oxirane as purine precursors)

RN 181022-34-4 ZCAPLUS  
CN Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro-, compd. with 2-chloro-4-nitro-1H-imidazole (1:1) (9CI) (CA INDEX NAME)

CM 1

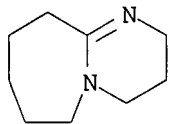
CRN 57531-37-0  
CMF C3 H2 Cl N3 O2



CM 2

CRN 6674-22-2

CMF C9 H16 N2

IT 549549-01-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

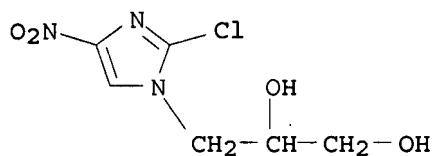
(preparation of (dihydroxypropyl)nitroimidazoles via addition of DBU-salts

of

nitroimidazoles to (hydroxymethyl)oxirane as purine precursors)

RN 549549-01-1 ZCAPLUS

CN 1,2-Propanediol, 3-(2-chloro-4-nitro-1H-imidazol-1-yl)- (9CI) (CA INDEX NAME)

IT 549549-02-2P 549549-03-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(stereoselective preparation of (dihydroxypropyl)nitroimidazoles via

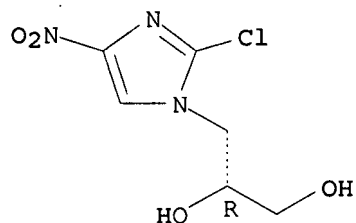
addition

of DBU-salts of nitroimidazoles to chiral (hydroxymethyl)oxirane as purine precursors)

RN 549549-02-2 ZCAPLUS

CN 1,2-Propanediol, 3-(2-chloro-4-nitro-1H-imidazol-1-yl)-, (2R)- (9CI) (CA INDEX NAME)

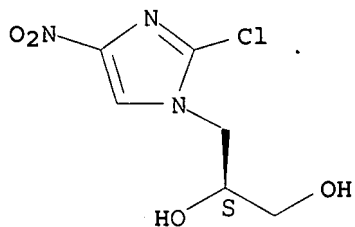
Absolute stereochemistry. Rotation (+).



RN 549549-03-3 ZCAPLUS

CN 1,2-Propanediol, 3-(2-chloro-4-nitro-1H-imidazol-1-yl)-, (2S)- (9CI) (CA  
INDEX NAME)

Absolute stereochemistry. Rotation (-).



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